CSC's services for researchers

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HPC support

Outline

- What is CSC?
- CSC computing services
- CSC data management services
- Support services
- Getting started with CSC services

Non-profit state organization with special tasks

Turn over in 2019

51 M€

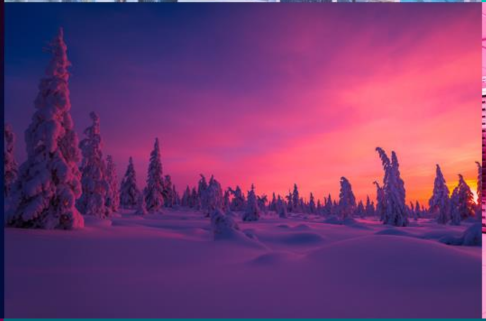
Headquarters in Espoo, datacenter in Kajaani

Owned by state (70%) and all Finnish higher education institutions **(30%)**

Circa **500** employees

Thanks to our agreement
with the Ministry of Education and Culture, our services targeted at researchers are largely free of charge!

Read more: *https://research.csc.fi/free-of-charge-use-cases*



CSC’s solutions


Computing and software


Data management and analytics for research


Support and training for research


Research administration


Solutions for managing and organizing education


Solutions for learners and teachers


Solutions for educational and teaching cooperation


Hosting services tailored to customers’ needs


Identity and authorisation


Management and use of data

ICT platforms, Funet network and data center functions are the base for our solutions

Our customers

Researchers,
research institutes and
organizations

Organizations providing
education

Memory organizations,
state and public
organizations

Support in all of the phases of a research process

Scientific drivers for CSC infrastructure

New challenges

Large scale simulations

- For example climate change, space weather, fusion reactors, astronomical phenomena, particle physics

Mid-scale simulations

- For example materials science, energy technology, GIS

Data-intensive computing

- For example computational econometrics, bioinformatics, language research

Data-intensive computing for sensitive data

- For example medical research, register research

Artificial intelligence

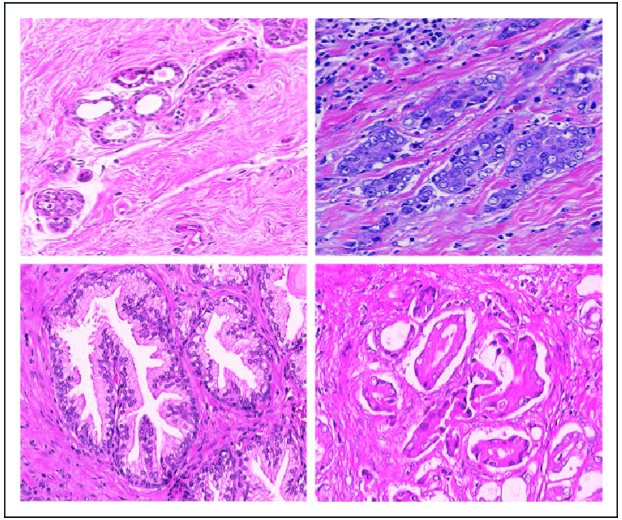
- For example natural language research, business applications, computer vision

Internet of Things (IoT) and data streams

- For example satellites, weather stations, sensor networks

Real-world examples – artificial intelligence

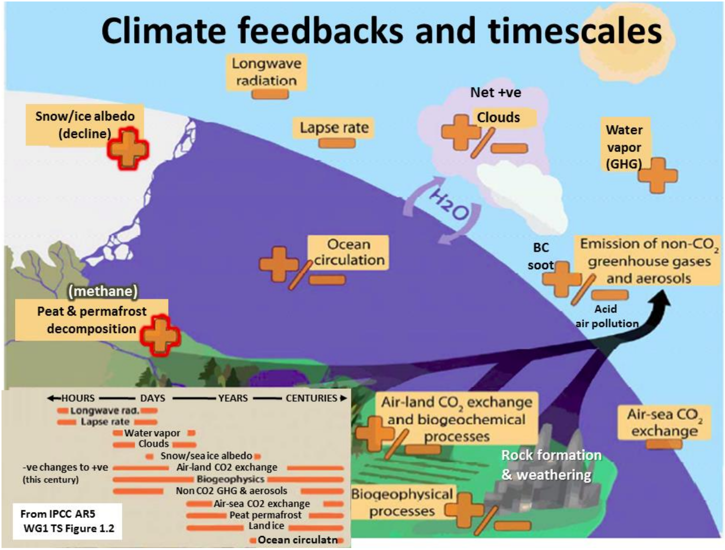
- Prediction of molecular phenotypes for cancer diagnosis
  - Molecular phenotyping can make diagnosis of breast cancer more precise and comprehensive
  - Deep neural networks are utilized for classification of histopathology image data
  - Large data volumes and optimized computational pipeline using both CPU and GPU computation
  - PI: Pekka Ruusuvuori, Tampere University



DOI: 10.1177/2374289518756306

Real-world examples - medium-scale simulations & data-intensive computing & data streams

- Atmospheric feedback mechanisms
  - In study of climate change, understanding feedback mechanisms is crucial for because they may either amplify or diminish the effect. Therefore these are key for determining the climate sensitivity and future climate.
  - This research involves various environmental measurements, satellite data and multiscale modelling. The multiscale models research start from nanoscale (quantum chemistry), reaching out towards global atmospheric models.
  - PI: Prof. Markku Kulmala, University of Helsinki

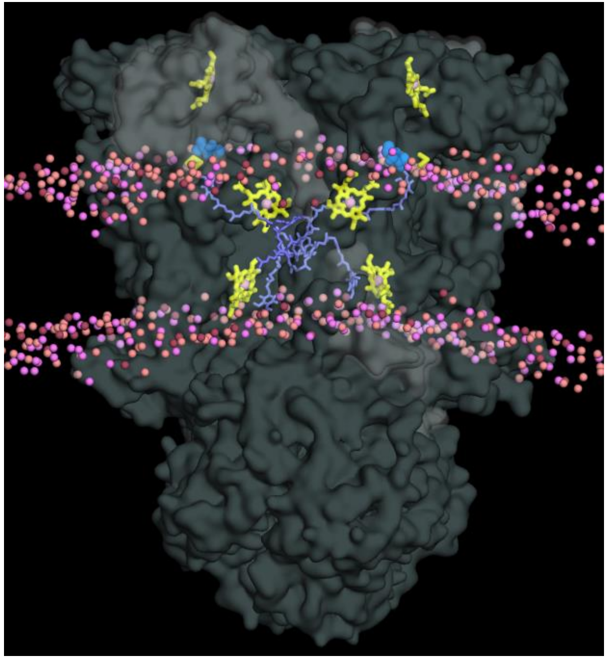


Real-world examples – medium scale simulations

- Spreading of aerosol particles in air
  - Computational fluid dynamics modelling of airborne transmission of coronavirus
  - Medium scale simulations with few hundred CPU cores
  - PI Ville Vuorinen, Aalto University

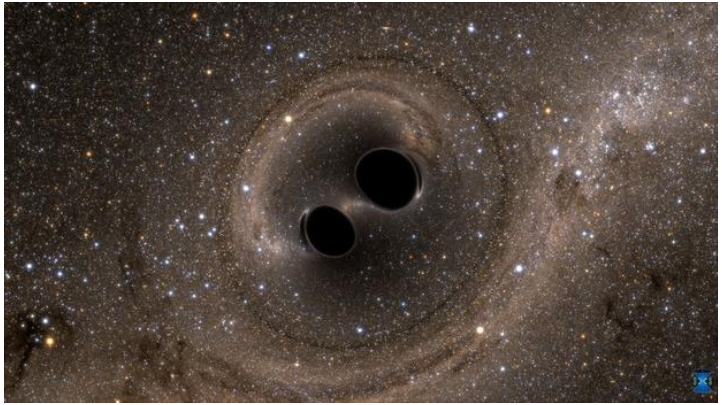
Real-world examples - medium-scale simulations

- Atomic level simulations of mitochondrial mutations
  - Molecular dynamic simulations of amino acid change and electron transfer during cellular respiration
  - New insight into GRACILE syndrome
  - Medium scale simulations with hundreds of CPU cores
  - PI: Vivek Sharma, University of Helsinki



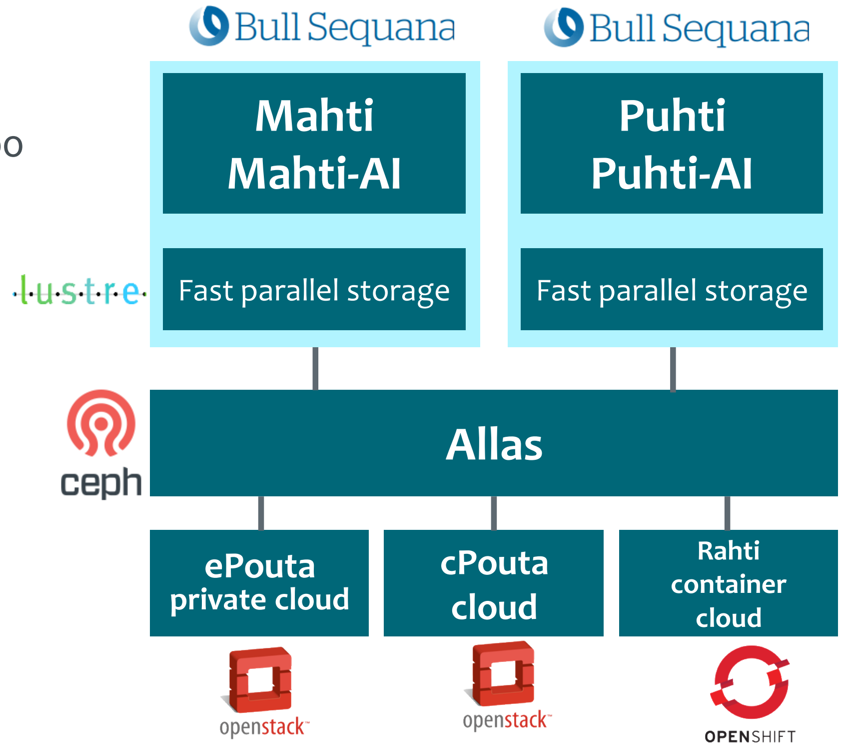
Real-world examples - large-scale simulations

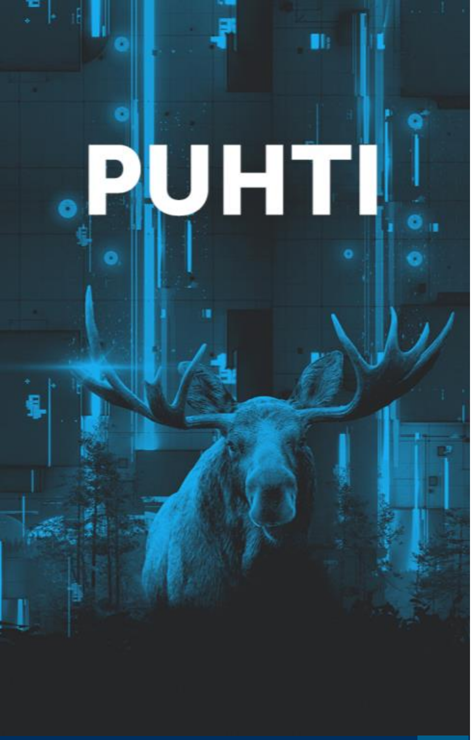
- Gravitational waves from early universe
  - Computational modeling of sources of gravitational waves
  - Phase transitions at Higgs boson “turning on” (10 picoseconds after Big Bang)
  - Large simulations with over ten thousand CPU cores
  - PI: David Weir, University of Helsinki



Balanced Compute and Data ecosystem

- **Supercomputers: Puhti and Mahti**
  - **Puhti** - Supercomputer with Intel CPUs & V100 GPUs(2019)
  - **Mahti** - Supercomputer with AMD CPUs and A100 GPUs (2020/2021)
- **Cloud services**
  - **Pouta** and **Rahti**
- **Object storage service: Allas**
  - New service for computing and cloud services, data can be shared to Internet
- **When you need even more**
  - PRACE research infrastructure & LUMI





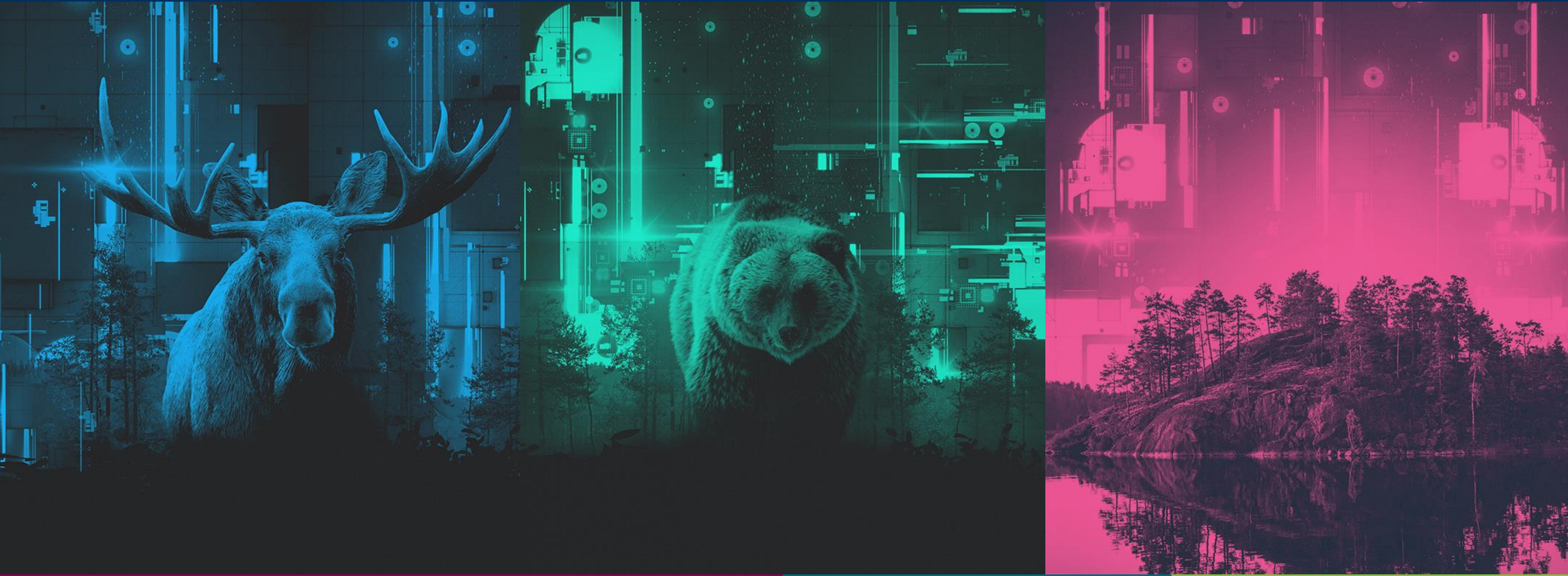
Puhti Supercomputer

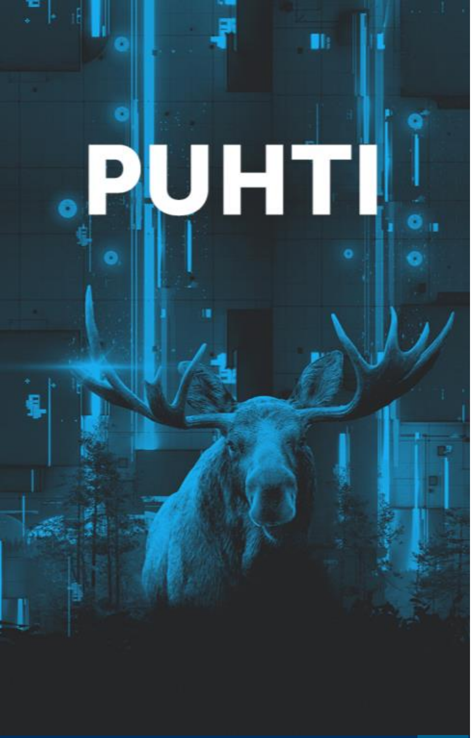
- Atos BullSequana X400 cluster based on Intel CPUs
- 700 CPU nodes with a range of memory sizes and local storage options, all connected with a fast interconnect.
- Reserve compute and memory resources flexibly and run anything from interactive single core data processing to medium scale simulations spanning multiple nodes.
- 80 GPU nodes (320 GPUs) suitable for all kinds workloads capable of utilizing GPUs, even heavy AI models that span multiple nodes.
- Puhti has wide selection of scientific software installed.
- 4.8 PB Lustre file system

Mahti Supercomputer

- Massively parallel jobs requiring large floating point performance and capable interconnect – 9,5 petaflops!
- 1404 nodes (7,5 petaflops). Each node has two AMD Rome 7H12 CPUs with 64 cores each at 2.6 GHz
- 24 GPU nodes (2,0 petaflops) are equipped with 512 GB of memory, a local 3,8 TB Nvme drive and four Nvidia Ampere A100 GPUs.
- Jobs use always full nodes for maximum performance, interactive use on Mahti allows also less
- Over 8 petabytes of work disk for data under active use

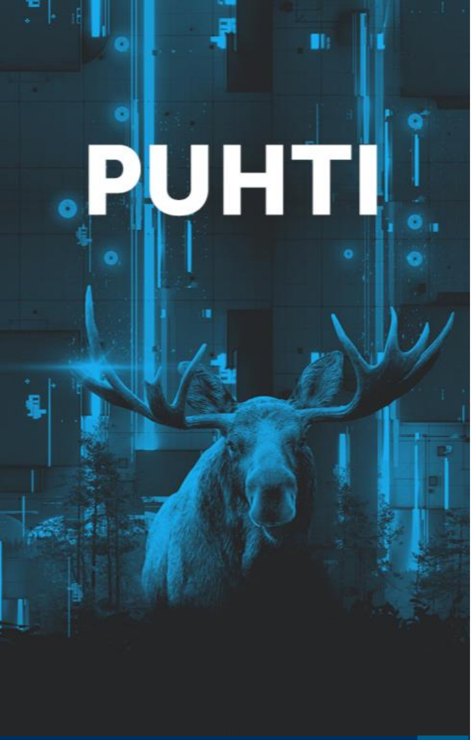
Technical details





Puhti Supercomputer

- Supports wide range of use cases
- Powerful CPU partition with ~700 nodes
  - Range of memory sizes and storage options
  - Fast interconnect between nodes
- Workloads from interactive single core data processing to medium scale multiple node simulations
- 80 GPU nodes with total of 320 GPUs
  - AI and other workloads with GPUs
  - Also heavy AI models spanning multiple nodes
- 4 Petabytes work disk for data under active use



Technical specifications

	CPU	CPU cores	Memory	Number of nodes
Puhti CPU parition	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	192 GB	532
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	384 GB	92
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	384 GB + 3.2 TB NVMe	40
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	768 GB	12
	Xeon Gold 6230	2 x 20 cores @ 2.1 GHz	1.5TB	6
Puhti-AI GPU partition	Xeon Gold 6230 4 x V100 32 GB	2 x 20 cores @ 2.1 GHz	384 GB (Host) 128 GB (GPUs) 3.2 TB NVMe	80

- Infiniband HDR interconnect between nodes
  - 100 Gb/s in CPU partition, 200 Gb/s in GPU partition

Mahti Supercomputer

- Massively parallel jobs requiring large floating point performance and capable interconnect
  - In principle jobs can scale across full system
  - Also smaller parallel workloads
- Jobs use always full nodes for maximum performance
- Over 8 petabytes of work disk for data under active use

Technical specifications

- 1404 compute nodes with next generation AMD Rome CPUs
  - Two 64 core AMD EPYC 7H12 processors per node
  - 2.6 GHz base frequency (maximum boost 3.3 GHz)
  - 256 GB of memory per node
  - About 180 000 cores in total
- 24 GPU nodes with 4 NVIDIA A100 GPU cards each
- Infiniband HDR interconnect between nodes
  - 200 GB/s bandwidth
- Theoretical peak performance 7.5 Pflop/s

CSC's Cloud Services

- IaaS Cloud
  - User supplies a virtual machine (VM) image
  - Services accessible over internet
- WebUI, CLI & Rest APIs supported

cPouta

openstack

- IaaS Cloud for Sensitive Data Processing
  - Services accessible only from customer network
- WebUI, CLI & Rest APIs supported

ePouta

openstack

- PaaS Cloud
  - User supplies Docker container
  - Services accessible over internet
- In Closed Beta Phase
- WebUI, CLI & Rest APIs supported

Rahti

OPENSHIFT

- Different hardware flavours (hpc, GPU, I/O, ...) available for all cloud services

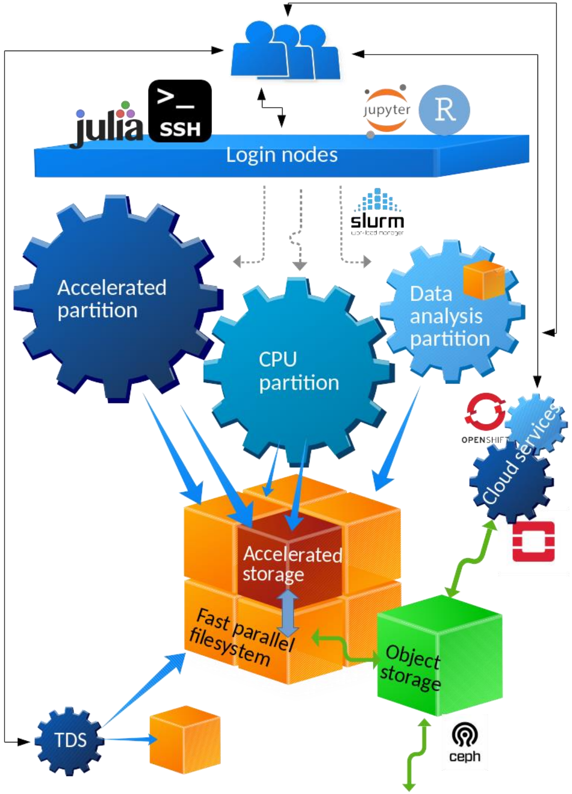
Programming for CSC supercomputers

- **Fortran, C++/C, Python, R, Julia, …**
- Parallel programming with MPI and OpenMP
  - Hybrid MPI + OpenMP becoming more important in Mahti
- Vectorization important for single CPU performance
- High performance libraries
  - BLAS, LAPACK, ScaLAPACK, FFTW, …
- GPU programming with OpenACC and CUDA
- Various frameworks for machine learning workloads
  - Keras, Tensorflow, PyTorch, …


LUMI
EuroHPC system of the North

LUMI – world leading pre-exascale system

- Consortium lead by CSC
  - Belgium, Czech Republic, Denmark, Estonia, Norway, Poland, Sweden and Switzerland
- 552 Pflop/s of peak performance
  - AMD CPUs and AMD GPUs
  - Highly capable I/O system
- 25 % of the resource dedicated to Finnish users
- To be hosted in Kajaani datacenter
- Available for customers in 2021



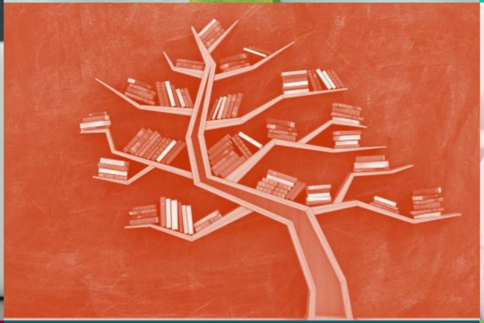
How to prepare for Lumi?

- LUMI is both huge possibility and huge challenge
  - Order of magnitude larger performance increase than normally with new CSC supercomputers (Mahti ~ 4 x Sisu, LUMI ~ 30 x Mahti)
  - Paradigm shift: fully accelerated system
- Thinking projects and use cases for Lumi
  - Cases for Tier-0 grand challenges
  - Existing GPU enabled applications
  - Combining simulation and AI methods within the same workflow
- Modernizing applications and GPU-enabling them
  - "even if it works, fix it"

Programming models for Lumi

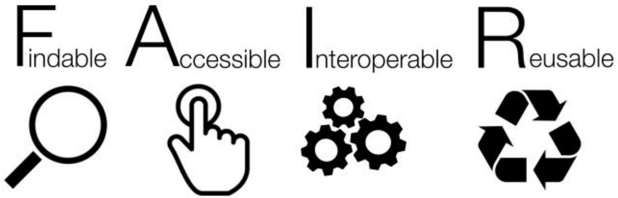
- **Fortran and C++** most important programming languages
  - **Python**, **R** and **Julia** will likely have a major role in workflow management and as ”driver” language
- MPI remains fundamental distributed memory approach
  - OpenMP and various GPU progamming approaches within a node
- GPU programming
  - **HIP**
  - **OpenMP5 (+ OpenACC)**
  - High-level libraries and frameworks (SYCL, Kokkos, RAJA,...)
  - Language-native GPU support (`std::for_each_n`, `do concurrent`)

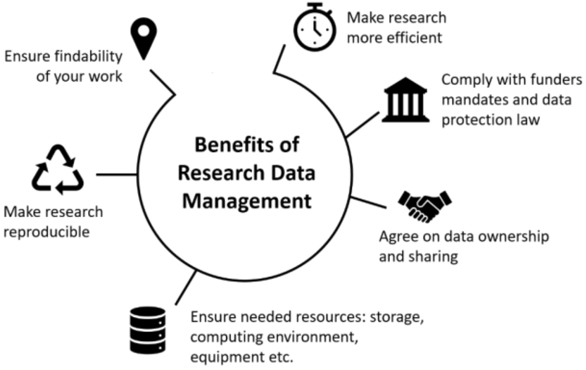
Data management services



Data Management

- Good data management is crucial for facilitating data sharing and ensuring the sustainability and accessibility of data in the long-term and therefore their re-use for future science.
- CSC has multiple options for storing data while you work on it and later on during the data lifecycle.





Research data storage Allas

- A storage site for any large datasets in the CSC environment. Can be used both for static research data and to collect and host cumulating or changing data.
- General use is free of charge based on users affiliation to a Finnish higher education institution or a state research institute. Default storage quota: 10 TB. Can be increased upon request. Projects with big amounts of data or where Allas is used as an application platform must agree separately with CSC.
- Data management is the responsibility of the users . The OpenStack Horizon web interface provides easy-to-use basic functions for data management and in the computing environment (Puhti/Mahti), there are ready-to-use tools to access Allas.
- Can be accessed on the CSC servers as well as from anywhere on the internet. It comes with the *S3* and *Swift* interfaces on a *CEPH* storage.
- SLA is intended and dimensioned for research (e.g. no backup).
- Storing data in Allas consumes *billing units*. The rate is 1 BU/TiBh, i.e. 1 TB of data stored in Allas consumes 24 BU in a day and 8760 BU in a year. Unlike most other object storage providers, CSC does not charge for object storage network transfers or API calls.

EUDAT Data Infrastructure

- EUDAT CDI (Collaborative Data Infrastructure) is a European consortium providing data management services for research.
- Origin in CSC lead EU projects
- More information:
  - www.eudat.eu

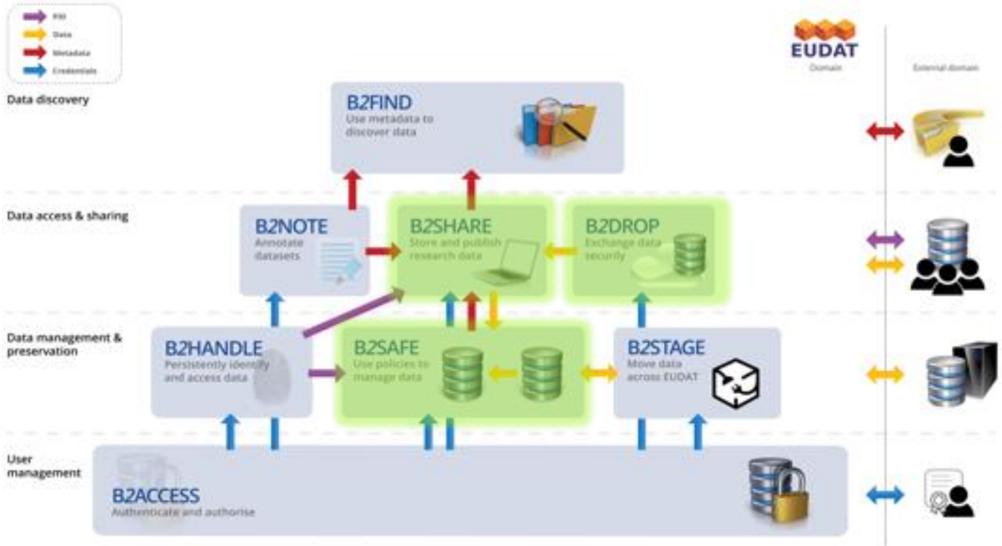
EUDAT CDI members

EUDAT Services at CSC

- CSC provides customized data management solutions based on open EUDAT services.
- **B2SHARE**: Service to store, describe and publish research datasets
  - Generic and/or domain-specific metadata; harvested to B2FIND metadata search; DOI
  - Open version: b2share.eudat.eu (FI)
- **B2DROP**: Service to easily store and share data
  - Common space for teams, projects or organizations
  - Open version: b2drop.eudat.eu (DE)
- **B2SAFE**: Scalable data storage, replication and management service
  - Enables policy-based storage and replication across data centres

EUDAT Services at CSC

B2SHARE Store and Publish Research Data | B2DROP Synch and Share Research Data | B2SAFE Replicate Research Data Safely



EUDAT CDI Services Suite

Fairdata services promote transparency in research and science

- Fairdata.fi services help you to make your data FAIR:
  - You get secure storage for your research data and related materials
  - You can describe your data, regardless of where it's stored. Dataset metadata is also harvested to Fairdata and from Fairdata to other services
  - You can publish your dataset and get a persistent identifier (URN or DOI) for it, enabling citations. You can set your published research data openly accessible or restrict the access.
  - You can explore and download research datasets created by others
  - Datasets can be transferred to digital preservation service (Fairdata DPS)

Fairdata services

- To use the services
  - Register a CSC account to describe and publish your data using Qvain and Etsin. Storing data in IDA requires project-specific storage space, which is granted by your home organization
  - Long term preservation (Fairdata DPS) requires a contract.
- What Fairdata is not suitable for
  - Sensitive personal data is not eligible for Fairdata IDA service
  - Availability of metadata or data cannot be limited for e.g. organization's internal use

Suitable for all digital research material and related metadata

Free of charge for users in Finnish higher education institutions and research institutes

CSC

IDA

Data stored in IDA

Data stored outside of Fairdata

↓

Qvain

Describe your dataset, publish it and get a persistent identifier.

↓

Etsin

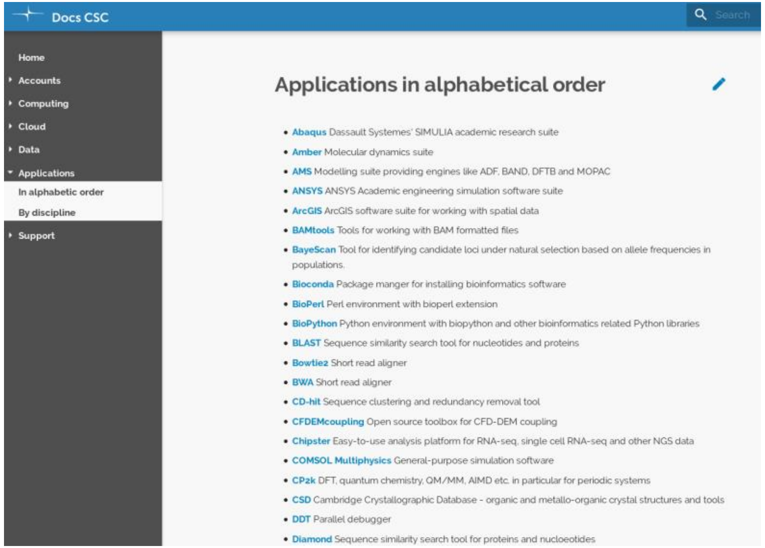
DOI
URN

Your dataset can be discovered and downloaded in Etsin.

Support services for researchers

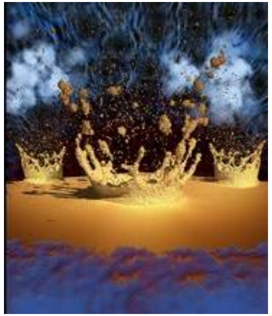
Software

- CSC provides researchers the largest collection of scientific software and databases in Finland.
- The list of pre-installed and supported scientific software packages can be found at: https://research.csc.fi/software
- Users can install also their own applications
  - CSC can provide support



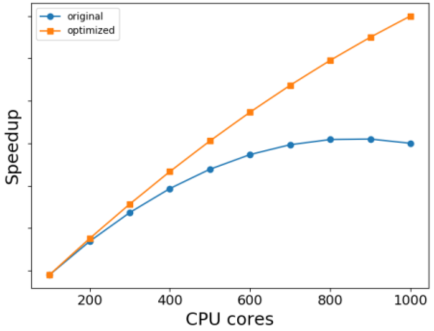
Expert Support in Sciences and Methods

- Help customers to select the most suitable and effective tools and software for each research project
- Advise in the effective use of supercomputers and cloud computation
- Support in optimisation and parallelisation of your own applications
- In-house scientific software development
  - Elmer, Chipster
- Advise in using and applying for international resources
- Ask for support from CSC Service Desk **servicedesk@csc.fi**



Optimization service

- Help CSC's users to improve their HPC software
  - Consulting discourse between an application developer and CSC's specialist
- Suitable development projects
  - Code optimization i.e., improving single-core and parallel efficiency of the application
  - Parallelization of a serial code
  - Reduction of memory and/or I/O requirements of the application
  - Conversion of an MPI application into a hybrid MPI+OpenMP application
  - Enabling the use of the accelerator technologies such as graphic processing units (GPU).
- Send a free-form description of your case to **servicedesk@csc.fi**



Training services

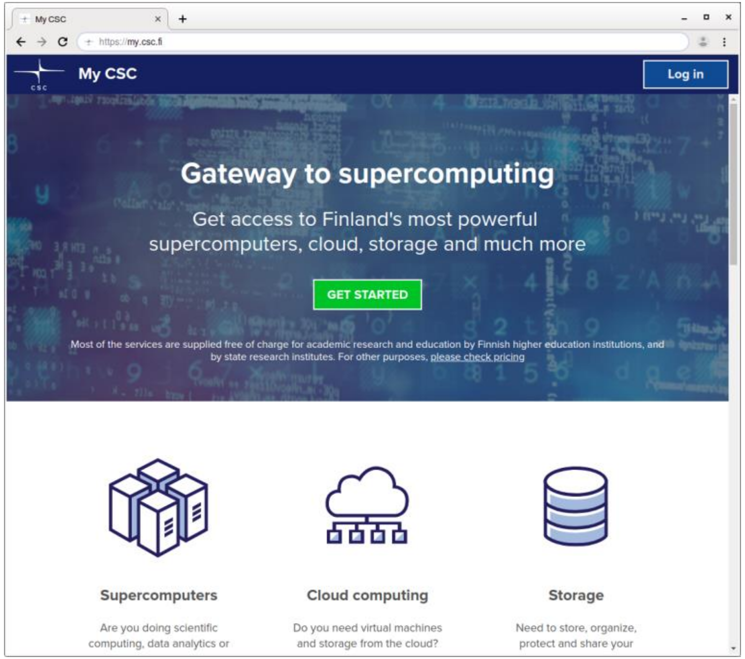
- Annually about 70 training events for Finnish universities and research institutes: courses, workshops, seminars and webinars
- Lecturers and trainers are leading experts
- Training aimed to familiarize you with the CSC infrastructure and its efficient use
- Courses can be customized according to your needs
- Information and registration for upcoming trainings and learning materials can be found in **CSC's training portal** www.csc.fi/training
- If you have questions related to CSC's training services, contact **courses@csc.fi**

How to get access?



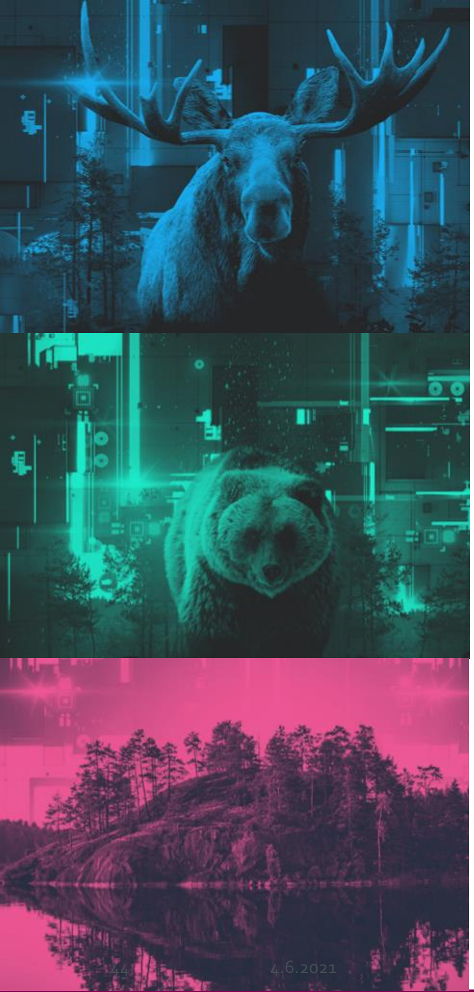

How to get access?

- **Your Haka user ID is your access to more than 160 services.**
  - Web based services ready to use
  - Register at [my.csc.fi](my.csc.fi) to get a personal CSC user account
  - If your organization does not have Haka, contact servicedesk@csc.fi
  - Project supervisor applies for resources and services, and can invite other people to projects
  - Instructions https://research.csc.fi/accounts-and-projects
- **Customer service**
  - Support and guidance **servicedesk@csc.fi**
  - Weekdays 8.30–16.00.



When to use CSC services ?

- Single core / single GPU performance not necessarily much different from local workstation or FCGI systems, but added value possibly from:
- Software available in CSC supercomputers
- More memory in CSC supercomputers (up to 1.5 TB)
- Parallel computations with more resources than in local systems
- Moving between different systems should be relatively easy
  - Similar **module** and **batch** system (**Slurm**)



Questions?

Information about CSC in general: www.csc.fi

Information for researchers: research.csc.fi

User documentation: docs.csc.fi